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EPR and optical spectra of Yb3+ in CsCdBr3: Charge-transfer effects on the energy-level structure of Yb3+ in the symmetrical pair centers

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Abstract

Electron paramagnetic resonance (EPR), optical absorption, fluorescence, and excitation spectra of CsCdBr3:1% Yb3+ single crystals were taken at 4.2 K. An analysis of the dependence of the EPR spectrum on the magnetic-field direction and a comparison of the recorded signal shapes with simulated envelopes over the magnetic dipole transitions of the expected dimers containing all ytterbium isotopes were performed. This allowed us to assign the measured EPR spectra unambiguously to the symmetrical pair center of the type Yb3+-Cd2+ vacancy-Yb3+ substituting for three adjacent Cd2+ ions in the bromine octahedra chain. A distance of 0.596 nm between the magnetically equivalent Yb3+ ions was determined from the line splitting due to magnetic dipole-dipole interaction. An interpretation of the optical spectra in compounds containing (YbBr6)3- complexes is presented, which is based on a crystal-field theory accounting for an interaction between the ground 4f13(Yb3+)[4p6(Br-)]6 and excited 4f14(Yb2+)4p5(Br)[4p 6(Br-]5 charge-transfer configurations. The observed large splitting of the excited 2F5/2(4f13) crystal-field multiplet is explained on the basis of a quasiresonant hybridization of the 4f-hole state with the spin orbitals of the charge-transfer states. With physically reasonable values of the fitted model parameters, the calculated energy level diagram of the 4f13 configuration and the g tensor of the Yb3+ ion in the crystal-field ground state are in good agreement with the experimental data.

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